

FIG. 1

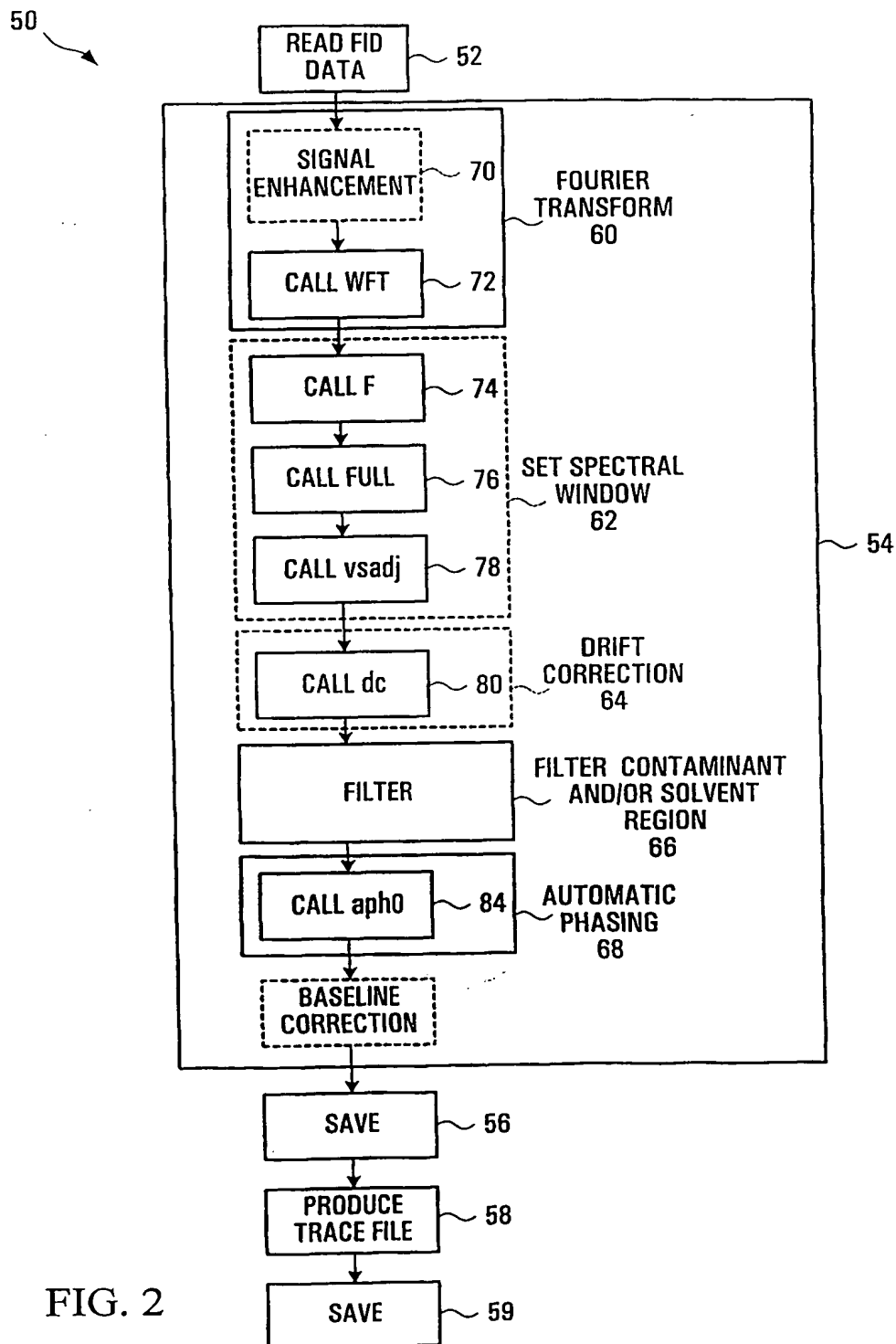
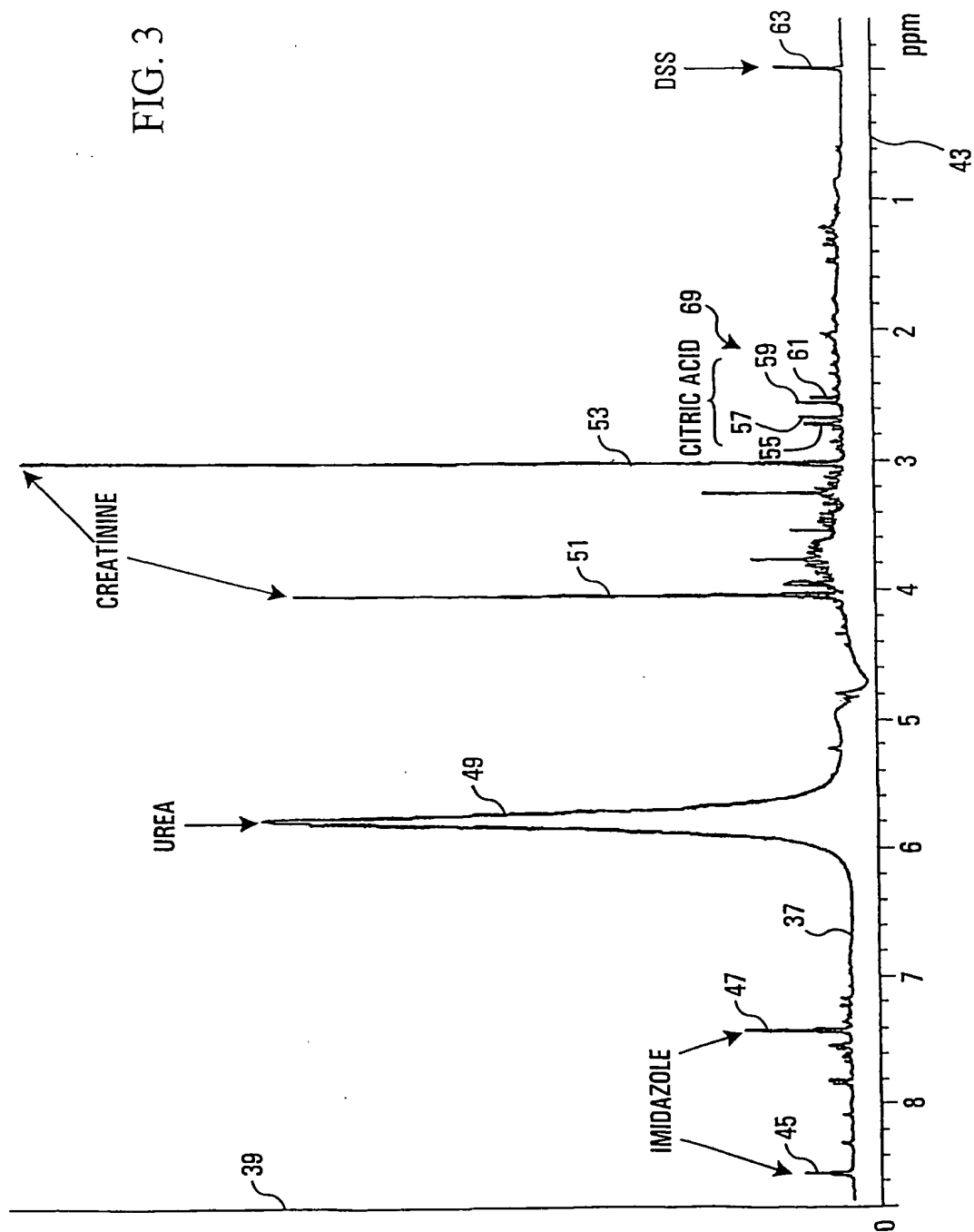


FIG. 2



FILTER SELECTED REGION

66

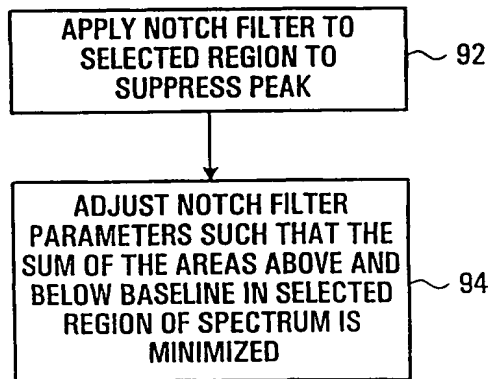


FIG. 4

**PROCESS FOR IDENTIFYING
COMPOUNDS FROM A TEST
SPECTRUM**

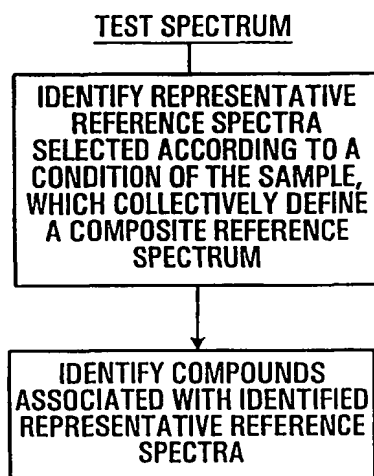
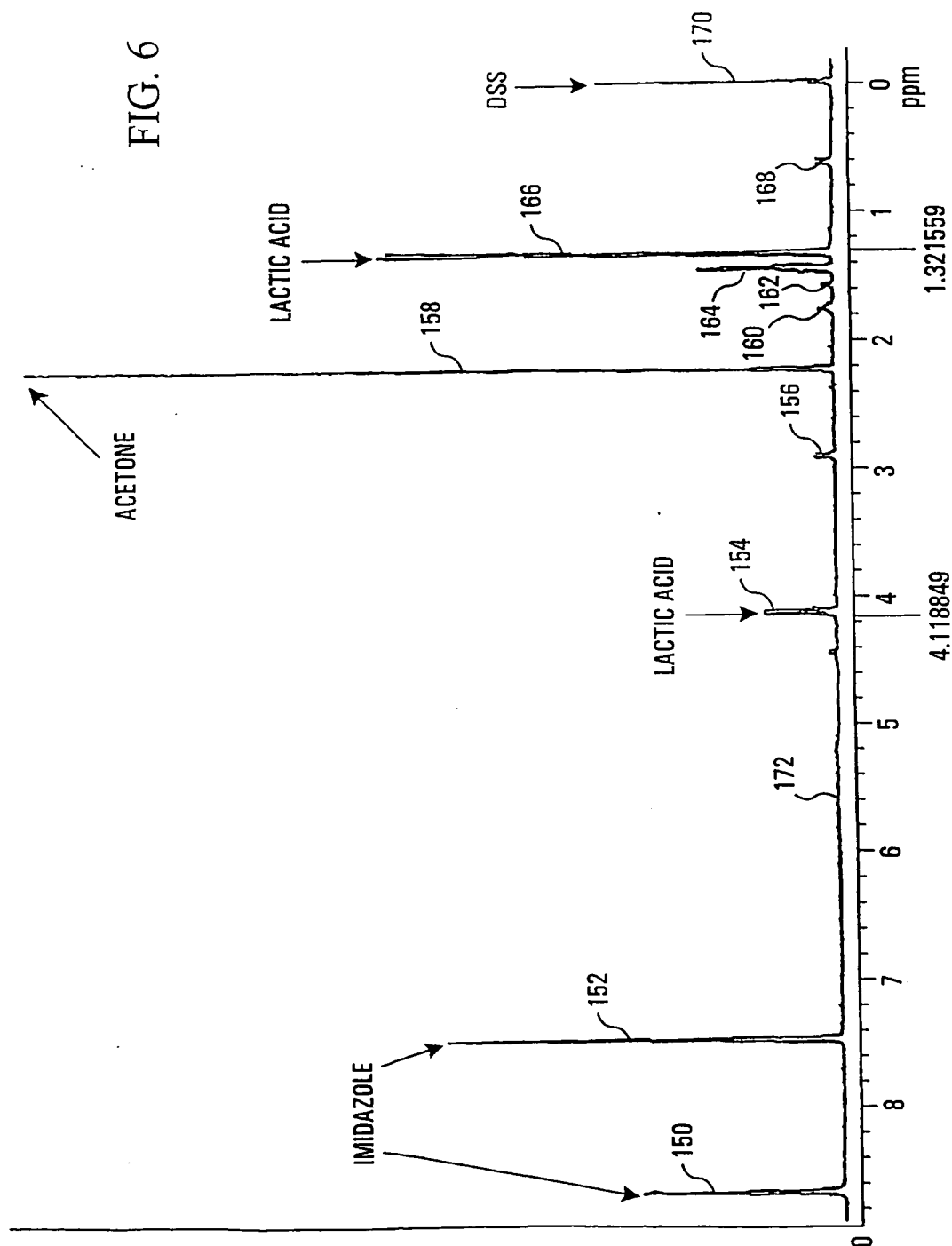


FIG. 5



REAL SPECTRAL DATA · pH=5.10

```

< ?xml version = "1.0"? >
< !-compoundDB version = "2.0".. >
< compound >
  < name > LacticAcid < /name >
  < molecularWeight > 90.08 < /molecularWeight >

  < experiment >
    < pH > 5.1 < /pH >
    < temperatureKelvin > 298.150000 < /temperatureKelvin >
    < DSSRatio > 0.533668 < /DSSRatio >
    < concentration > 4.308710 < /concentration >
    < timestamp > Sept 5 2001 < /timestamp >
    < sourceFID > lacticacid.fid < /sourceFID >
    < magnetMHz > 400.120773 < /magnetMHz >
    < spectralWidthHz > 6006.006006 < /spectralWidthHz >
  < /experiment >

  < cluster >
    210 → < protonNumber > 3 < /protonNumber >
    212 → < quantification > 1 < /quantification >
    < subCluster >
      214 → < centerPPM > 1.321559 < /centerPPM >
      < lorentzianWidthAdjust > 2.893258 < /lorentzianWidthAdjust >
      < peak >
        220 → < offsetCenterHz > -3.455480 < /offsetCenterHz >
        222 → < height > 0.988680 < /height >
        224 → < protonRatio > 1.491461 < /protonRatio >
      < /peak >
      < peak >
        < offsetCenterHz > 3.455480 < /offsetCenterHz >
        < height > 1.0000000 < /height >
        < protonRatio > 1.508539 < /protonRatio >
      < /peak >
    < /subCluster >
  < /cluster >

```

200

202

206

216

218

204

FIG. 7A

```

< cluster >
  < protonNumber > 1 < /protonNumber >
  < quantification > 0 < /quantification >
  < subCluster >
    < centerPPM > 4.118849 < /centerPPM >
    < lorentzianWidthAdjust > 13.441432 < lorentzianWidthAdjust >
    < peak >
      < offsetCenterHz > -10.366999 < /offsetCenterHz >
      < height > 0.057244 < /height >
      < protonRatio > 0.130861 < /protonRatio >
    < /peak >
    < peak >
      < offsetCenterHz > -3.43221144 < /offsetCenterHz >
      < height > 0.164751 < /height >
      < protonRatio > 0.376629 < /protonRatio >
    < /peak >
    < peak >
      < offsetCenterHz > 3.487744 < /offsetCenterHz >
      < height > 0.161840 < /height >
      < protonRatio > 0.369975 < /protonRatio >
    < /peak >
    < peak >
      < offsetCenterHz > 10.366999 < /offsetCenterHz >
      < height > 0.053601 < /height >
      < protonRatio > 0.122535 < /protonRatio >
    < /peak >
  < /subCluster >
< /cluster >
< /compound >
  
```

208

204

FIG. 7B

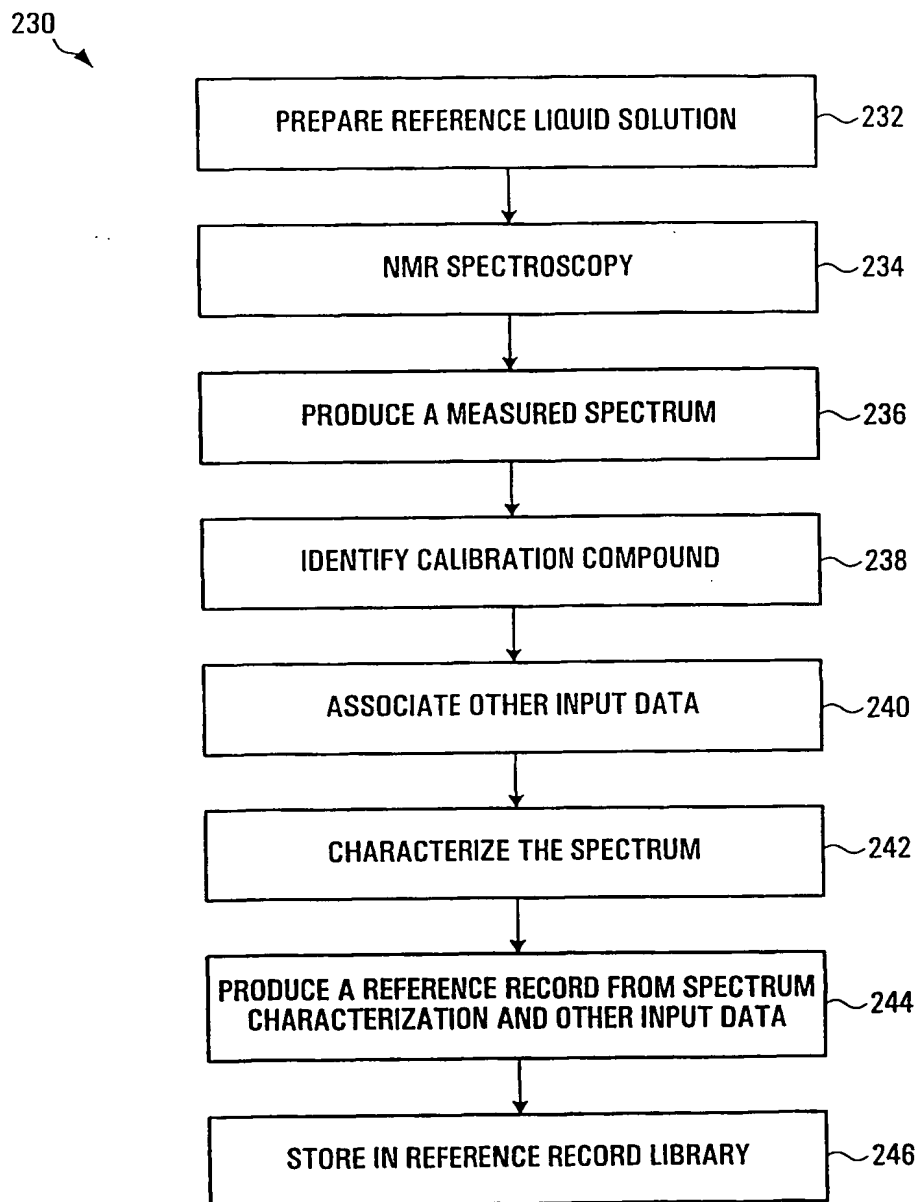


FIG. 8

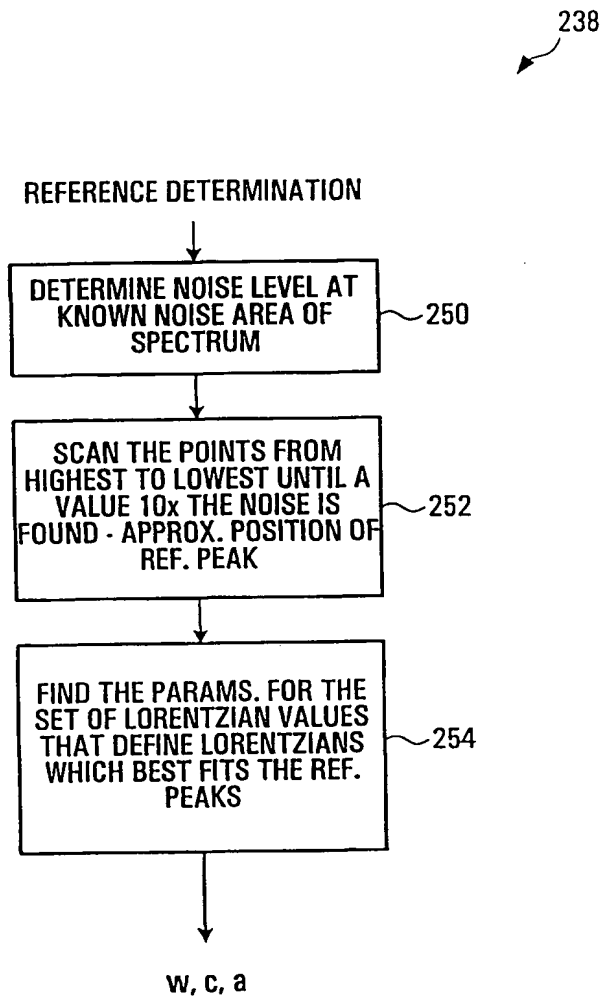


FIG. 9

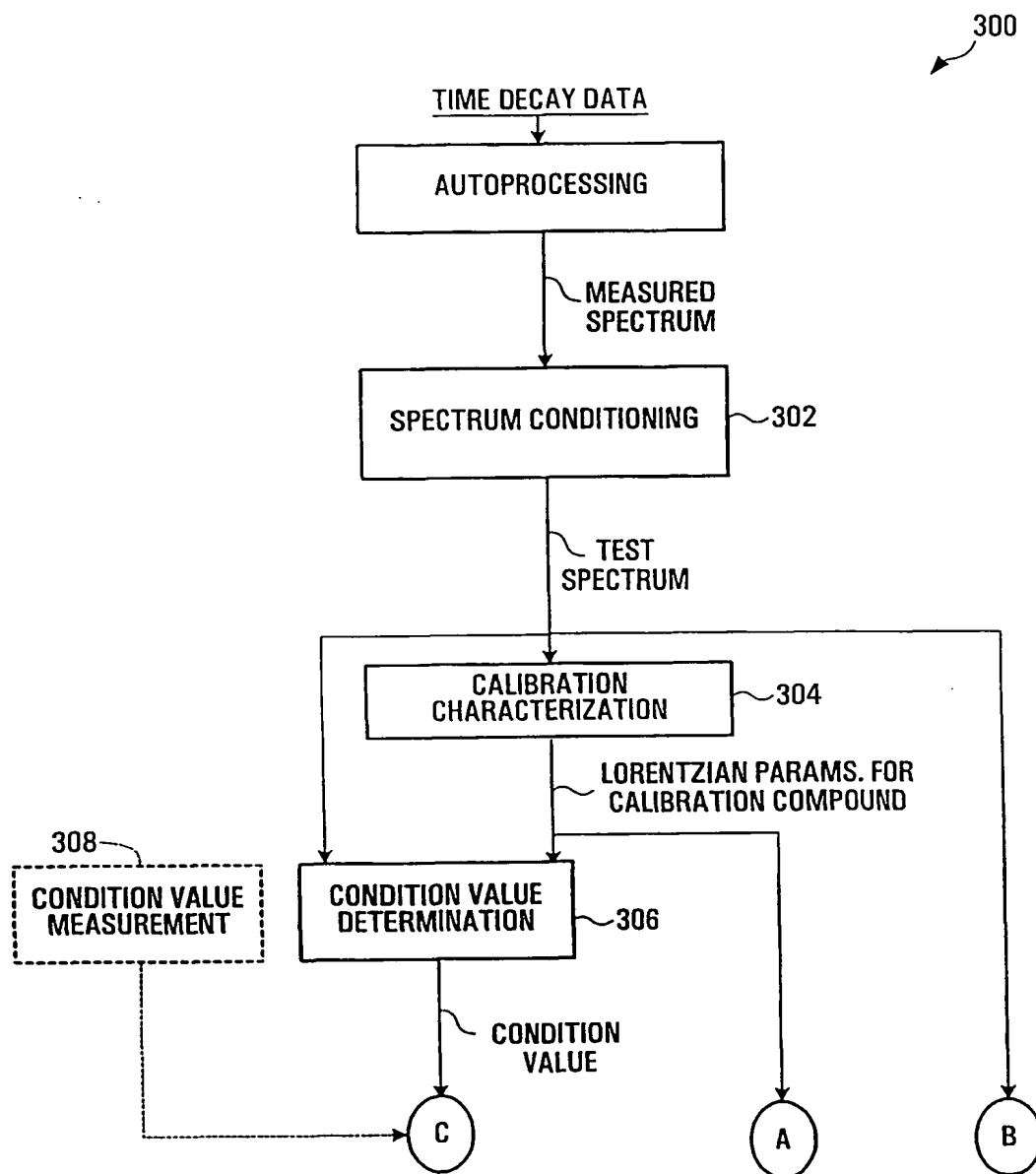


FIG. 10A

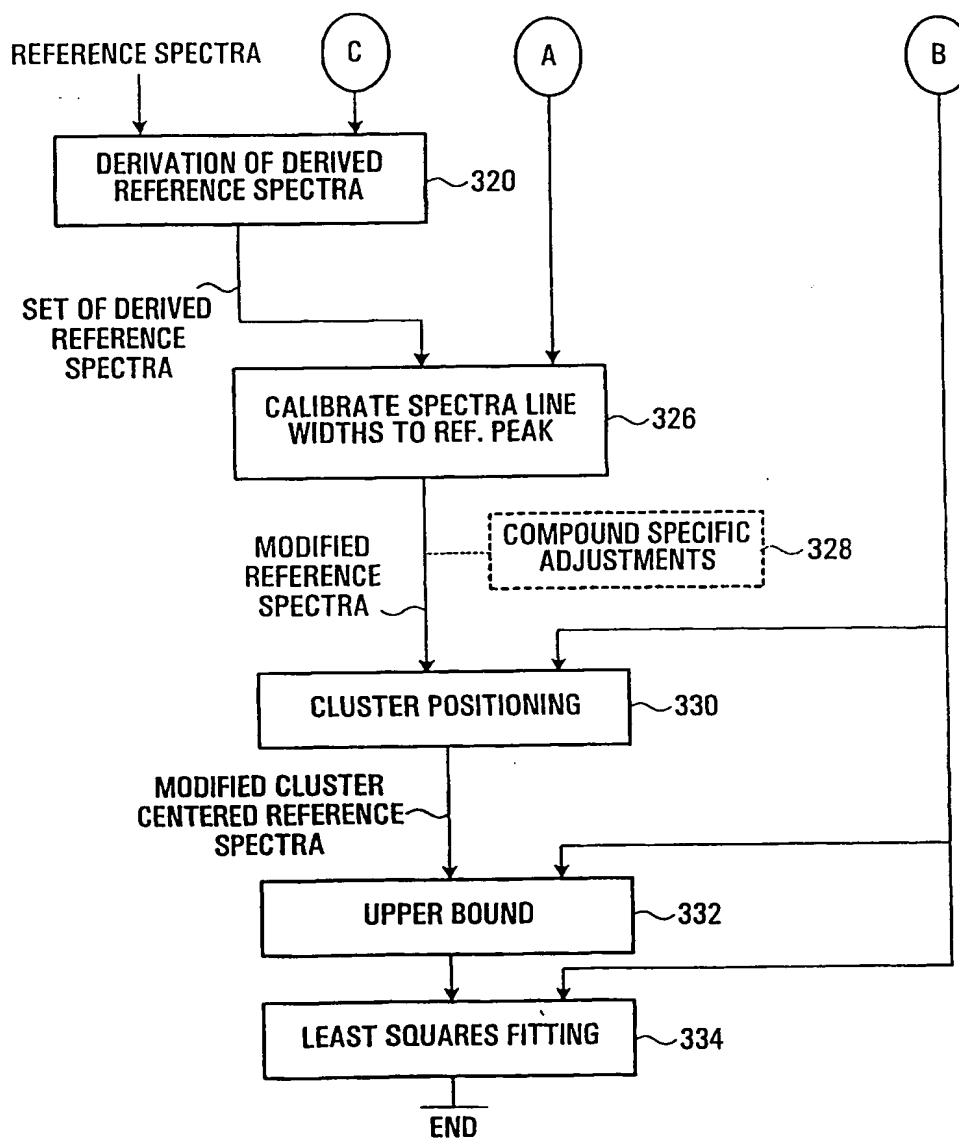


FIG. 10B

CONDITION VALUE DETERMINATION

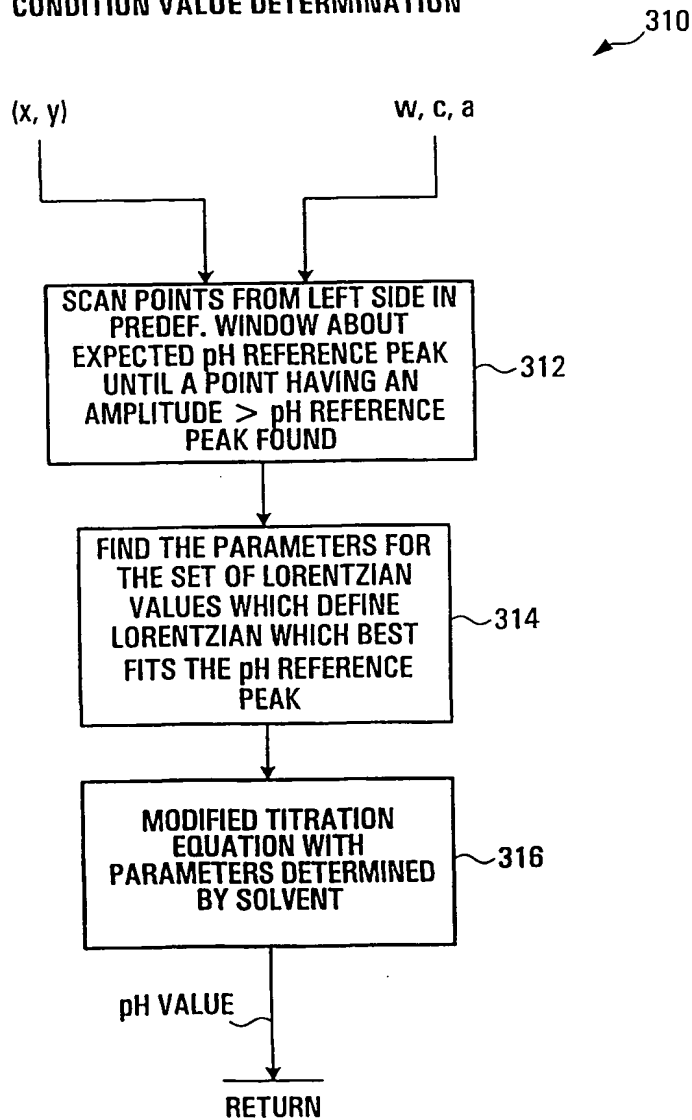


FIG. 11

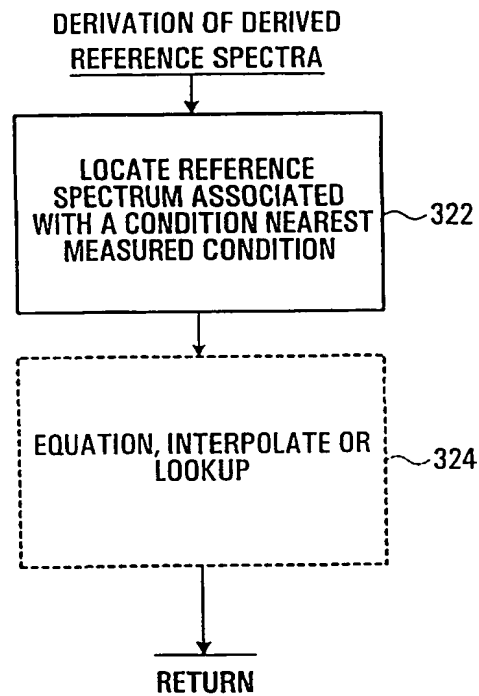


FIG. 12

Real Spectral Data - pH=5.45

```
<?xml version="1.0"?>
<!-- compoundDB version="2.0" -->
<compound>
  <name>LacticAcid</name>
  <molecularWeight>90.08</molecularWeight>

  <experiment>
    <pH>5.45</pH>
    <temperatureKelvin>298.150000</temperatureKelvin>
    <DSSRatio>0.533668</DSSRatio>
    <concentration>4.308710</concentration>
    <timestamp>Sept 5 2001</timestamp>
    <sourceFID>lacticacid.fid</sourceFID>
    <magnetMHz>400.120699</magnetMHz>
    <spectralWidthHz>6006.006006</spectralWidthHz>
  </experiment>

  <cluster>
    <protonNumber>3</protonNumber>
    <quantification>1</quantification>
    <subCluster>
      <centerPPM>1.318770</centerPPM>
      <lorentzianWidthAdjust>1.562004</lorentzianWidthAdjust>
      <peak>
        <offsetCenterHz>-3.453329</offsetCenterHz>
        <height>0.983656</height>
        <protonRatio>1.487641</protonRatio>
      </peak>
      <peak>
        <offsetCenterHz>3.453329</offsetCenterHz>
        <height>1.000000</height>
        <protonRatio>1.512359</protonRatio>
      </peak>
    </subCluster>
  </cluster>
```

FIG. 13A

```
<cluster>
  <protonNumber> 1 </protonNumber>
  <quantification> 0 </quantification>
  <subCluster>
    <centerPPM> 4.110990 </centerPPM>
    <lorentzianWidthAdjust> 7.044502 </lorentzianWidthAdjust>
    <peak>
      <offsetCenterHz> -10.371092 </offsetCenterHz>
      <height> 0.054671 </height>
      <protonRatio> 0.124148 </protonRatio>
    </peak>
    <peak>
      <offsetCenterHz> -3.448909 </offsetCenterHz>
      <height> 0.164509 </height>
      <protonRatio> 0.373572 </protonRatio>
    </peak>
    <peak>
      <offsetCenterHz> 3.456819 </offsetCenterHz>
      <height> 0.163879 </height>
      <protonRatio> 0.372141 </protonRatio>
    </peak>
    <peak>
      <offsetCenterHz> 10.371092 </offsetCenterHz>
      <height> 0.057309 </height>
      <protonRatio> 0.130139 </protonRatio>
    </peak>
  </subCluster>
</cluster>
</compound>
```

FIG. 13B

Interpolated Data - pH=5.28

```
<?xml version="1.0"?>
<!-- compoundDB version="2.0" -->
<compound>
  <name> LacticAcid </name>
  <molecularWeight> 90.08 </molecularWeight>

  <experiment>
    <pH> 5.45 </pH>
    <temperatureKelvin> 298.150000 </temperatureKelvin> : copied
    <DSSRatio> 0.533668 </DSSRatio>
    <concentration> 4.308710 </concentration>
    <timestamp> Sept 5 2001 </timestamp>
    <sourceFID> lacticacid.fid </sourceFID> :copied
    <magnetMHz> 400.120699 </magnetMHz>
    <spectralWidthHz> 6006.006006 </spectralWidthHz>
  </experiment>

  <cluster>
    <protonNumber> 3 </protonNumber>
    <quantification> 1 </quantification>
    <subCluster>
      <centerPPM> 1.3202 </centerPPM> : interpolated
      <lorentzianWidthAdjust> 1.562004 </lorentzianWidthAdjust>
      <peak>
        <offsetCenterHz> -3.453329 </offsetCenterHz>
        <height> 0.983656 </height>
        <protonRatio> 1.487641 </protonRatio>
      </peak>
      <peak>
        <offsetCenterHz> 3.453329 </offsetCenterHz>
        <height> 1.000000 </height>
        <protonRatio> 1.512359 </protonRatio>
      </peak>
    </subCluster>
  </cluster>
```

FIG. 14A

```

< cluster >
  < protonNumber > 1 < /protonNumber >
  < quantification > 0 < /quantification >
  < subCluster >
    < centerPPM > 4.1149 < /centerPPM > :interpolated
    < lorentzianWidthAdjust > 7.044502 < /lorentzianWidthAdjust >
    < peak >
      < offsetCenterHz > -10.371092 < /offsetCenterHz >
      < height > 0.054671 < /height >
      < protonRatio > 0.124148 < /protonRatio >
    < /peak >
    < peak >
      < offsetCenterHz > -3.448909 < /offsetCenterHz >
      < height > 0.164509 < /height >
      < protonRatio > 0.373572 < /protonRatio >
    < /peak >
    < peak >
      < offsetCenterHz > 3.456819 < /offsetCenterHz >
      < height > 0.163879 < /height >
      < protonRatio > 0.372141 < /protonRatio >
    < /peak >
    < peak >
      < offsetCenterHz > 10.371092 < /offsetCenterHz >
      < height > 0.057309 < /height >
      < protonRatio > 0.130139 < /protonRatio >
    < /peak >
  < /subCluster >
< /cluster >
< /compound >
  
```

FIG. 14B

Generic Lactic Acid record

```
<?xml version="1.0"?>
<!-- compoundDB version="2.0" -->
<compound>
  <name>LacticAcid</name>
  <molecularWeight>90.08</molecularWeight>

  <experiment>
    <pH>5.45</pH>
    <temperatureKelvin>298.150000</temperatureKelvin>
    <DSSRatio>0.533668</DSSRatio>
    <concentration>4.308710</concentration>
    <timestamp>Sept 5 2001</timestamp>
    <sourceFID>lacticacid.fid</sourceFID>
    <magnetMHz>400.120699</magnetMHz>
    <spectralWidthHz>6006.006006</spectralWidthHz>
  </experiment>

  <cluster>
    <protonNumber>3</protonNumber>
    <quantification>1</quantification>
    <subCluster>
      <centerPPM> $y=m_1(pH)+b_1$ </centerPPM>
      <lorentzianWidthAdjust>1.562004</lorentzianWidthAdjust>
      <peak>
        <offsetCenterHz>-3.453329</offsetCenterHz>
        <height>0.983656</height>
        <protonRatio>1.487641</protonRatio>
      </peak>
      <peak>
        <offsetCenterHz>3.453329</offsetCenterHz>
        <height>1.000000</height>
        <protonRatio>1.512359</protonRatio>
      </peak>
    </subCluster>
  </cluster>
```

FIG. 15A

```

<cluster>
  <protonNumber> 1 </protonNumber>
  <quantification> 0 </quantification>
  <subCluster>
    <centerPPM>  $y=m_2(\text{pH})+b_2$  </centerPPM>
    <lorentzianWidthAdjust> 7.044502 </lorentzianWidthAdjust>
    <peak>
      <offsetCenterHz> -10.371092 </offsetCenterHz>
      <height> 0.054671 </height>
      <protonRatio> 0.124148 </protonRatio>
    </peak>
    <peak>
      <offsetCenterHz> -3.448909 </offsetCenterHz>
      <height> 0.164509 </height>
      <protonRatio> 0.373572 </protonRatio>
    </peak>
    <peak>
      <offsetCenterHz> 3.456819 </offsetCenterHz>
      <height> 0.163879 </height>
      <protonRatio> 0.372141 </protonRatio>
    </peak>
    <peak>
      <offsetCenterHz> 10.371092 </offsetCenterHz>
      <height> 0.057309 </height>
      <protonRatio> 0.130139 </protonRatio>
    </peak>
  </subCluster>
</cluster>
</compound>

```

FIG. 15B

Generic Lactic Acid record with Lookup Table link

```
<?xml version="1.0"?>
<!-- compoundDB version="2.0" -->
<compound>
  <name>LacticAcid</name>
  <molecularWeight>90.08</molecularWeight>

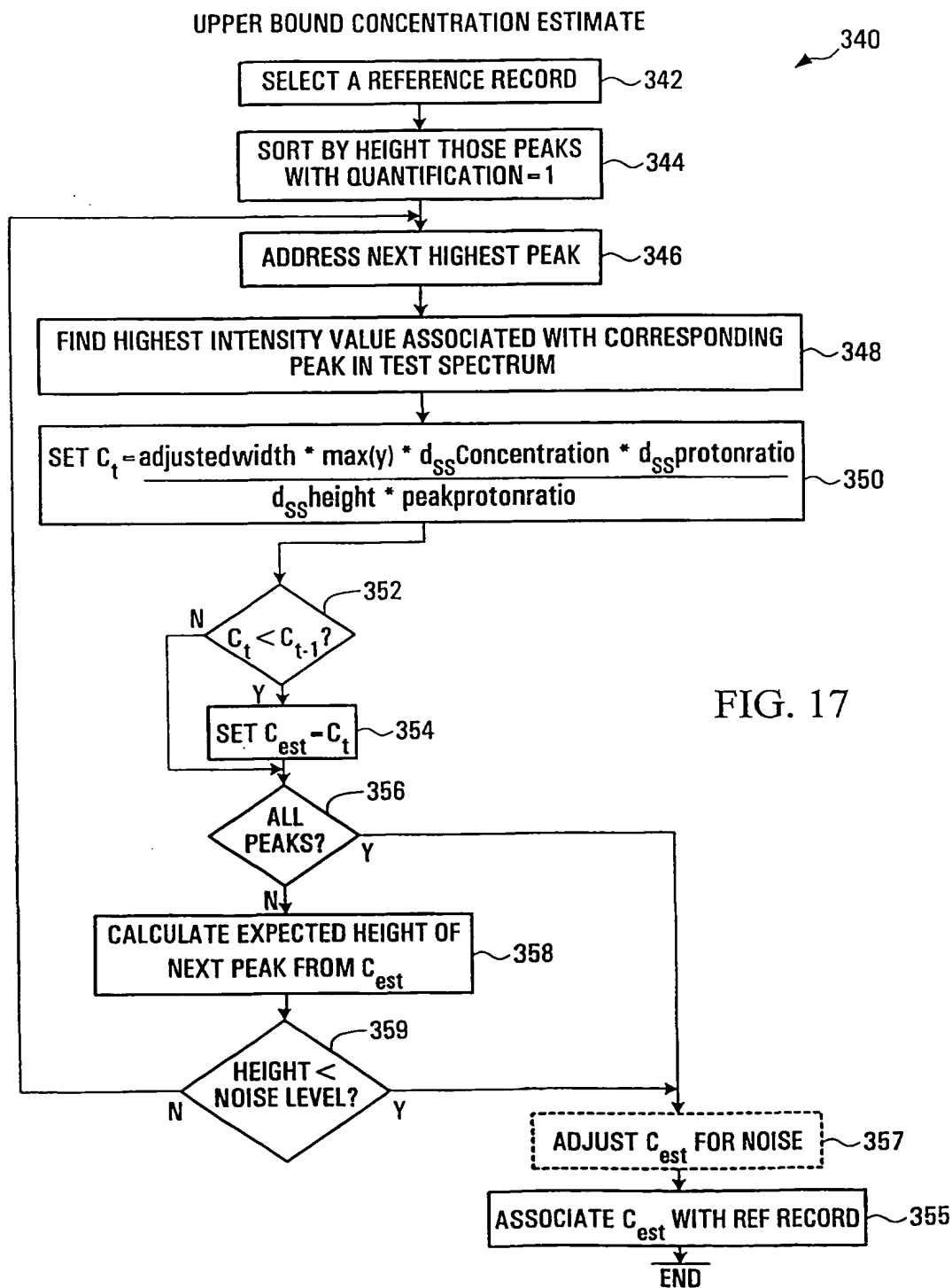
  <experiment>
    <pH>5.45</pH>
    <temperatureKelvin>298.150000</temperatureKelvin>
    <DSSRatio>0.533668</DSSRatio>
    <concentration>4.308710</concentration>
    <timestamp>Sept 5 2001</timestamp>
    <sourceFID>lacticacid.fid</sourceFID>
    <magnetMHz>400.120699</magnetMHz>
    <spectralWidthHz>6006.006006</spectralWidthHz>
  </experiment>

  <cluster>
    <protonNumber>3</protonNumber>
    <quantification>1</quantification>
    <subCluster>
      <centerPPM>LOOKUP TABLE LINK1</centerPPM>
      <lorentzianWidthAdjust>1.562004</lorentzianWidthAdjust>
      <peak>
        <offsetCenterHz>-3.453329</offsetCenterHz>
        <height>0.983656</height>
        <protonRatio>1.487641</protonRatio>
      </peak>
      <peak>
        <offsetCenterHz>3.453329</offsetCenterHz>
        <height>1.000000</height>
        <protonRatio>1.512359</protonRatio>
      </peak>
    </subCluster>
  </cluster>
```

FIG. 16A

```
<cluster>
  <protonNumber> 1 </protonNumber>
  <quantification> 0 </quantification>
  <subCluster>
    <centerPPM> LOOKUP TABLE LINK2 </centerPPM>
    <lorentzianWidthAdjust> 7.044502 </lorentzianWidthAdjust>
    <peak>
      <offsetCenterHz> -10.371092 </offsetCenterHz>
      <height> 0.054671 </height>
      <protonRatio> 0.124148 </protonRatio>
    </peak>
    <peak>
      <offsetCenterHz> -3.448909 </offsetCenterHz>
      <height> 0.164509 </height>
      <protonRatio> 0.373572 </protonRatio>
    </peak>
    <peak>
      <offsetCenterHz> 3.456819 </offsetCenterHz>
      <height> 0.163879 </height>
      <protonRatio> 0.372141 </protonRatio>
    </peak>
    <peak>
      <offsetCenterHz> 10.371092 </offsetCenterHz>
      <height> 0.057309 </height>
      <protonRatio> 0.130139 </protonRatio>
    </peak>
  </subCluster>
</cluster>
</compound>
```

FIG. 16B



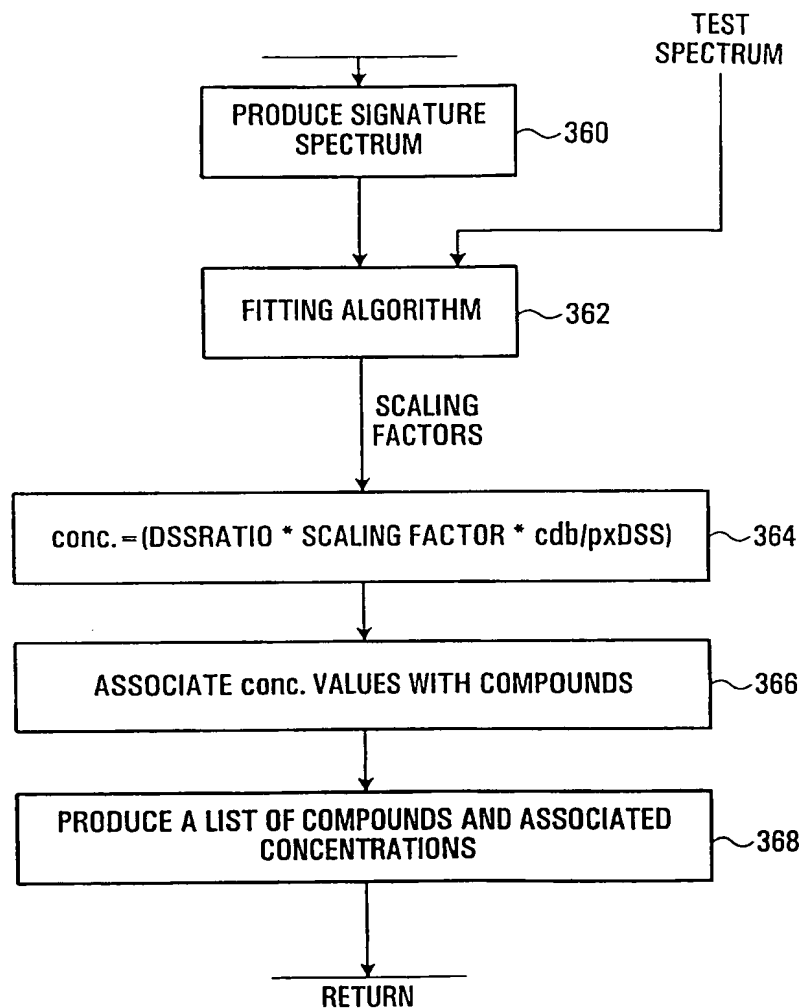


FIG. 18